

# Positron scattering from CH<sub>4</sub>, C<sub>2</sub>H<sub>4</sub> and C<sub>2</sub>H<sub>2</sub> with the Schwinger multichannel method implemented with a model potential

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As of recent years, theoretical groups have encountered difficulties to fully describe the experimental data on positron scattering by nonpolar molecules especially due the insufficient description of the positron-molecule correlation-polarization interactions in theoretical ab initio methods. As a consequence, there is no clear agreement between experimental and theoretical data.

The main problems are in the low energy regime (below 10 eV), in which the calculated data significantly underestimates the experimental results even when the Ps formation channel is closed. This can be associated with a lower than expected intensity of the calculated differential cross-sections in lower angles ( $\theta < 30^\circ$ ) and calculated bound state energies significantly smaller (if not identified as virtual states) than experimentally observed.

To further investigate the correlation-polarization description on positron scattering by molecules, we have included in the Schwinger multichannel codes the model potential of Swann and Gribakin [1-3]. They have adapted the model potential proposed by Mitroy and Ivanov [4] for positron-atom scattering to describe positron binding in molecules. Furthermore, Swann and Gribakin also employed the same model potential to calculate s-wave eigenphases for positron-molecule scattering.

In this work, we present calculated integral cross-sections, differential cross sections, s-wave eigenphases and virtual/bound state energies for the elastic positron scattering from methane (CH<sub>4</sub>), ethylene (C<sub>2</sub>H<sub>4</sub>) and acetylene (C<sub>2</sub>H<sub>2</sub>) with the SMC method [5,6] implemented with the model potential of reference [1]. The main reasons for choosing these molecules are due to their data availability and the fact that methane, ethylene and acetylene are the simplest alkane, alkene and alkyne, respectively, which make them ideal prototype molecules to study larger hydrocarbons. Also, they have received previous attention in reference [3] that could serve as a guide for later development. The results obtained by our calculations presented a much better agreement with existing experimental data for these molecules, especially when compared with the earlier calculations with the SMC method on the SP approximation.

## References

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